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(54) Title: A METHOD FOR PERFORMING RESTRAINED DYNAMICS DOCKING OF ONE OR MULTIPLE SUBSTRATES ON MULTI-SPECIFIC ENZYMES

(57) Abstract: The present invention relates to a method for performing restrained dynamics docking of one or several substrates having allosteric or synergistic effect on enzymes presenting multispecific and flexible active site. It also concerns a method for determining the 3D-substrates, which is the case for multispecific enzymes such as cytochrome P450, and specifically to cytochrome P450 3A4 and P450 3A7.